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* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS 1		Web Page for STN Seminar Schedule - N. America
NEWS 2	AUG 06	CAS REGISTRY enhanced with new experimental property tags
NEWS 3	AUG 06	FSTA enhanced with new thesaurus edition
NEWS 4	AUG 13	CA/CAplus enhanced with additional kind codes for granted patents
NEWS 5	AUG 20	CA/CAplus enhanced with CAS indexing in pre-1907 records
NEWS 6	AUG 27	Full-text patent databases enhanced with predefined patent family display formats from INPADOCDB
NEWS 7	AUG 27	USPATOLD now available on STN
NEWS 8	AUG 28	CAS REGISTRY enhanced with additional experimental spectral property data
NEWS 9	SEP 07	STN AnaVist, Version 2.0, now available with Derwent World Patents Index
NEWS 10	SEP 13	FORIS renamed to SOFIS
NEWS 11	SEP 13	INPADOCDB enhanced with monthly SDI frequency
NEWS 12	SEP 17	CA/CAplus enhanced with printed CA page images from 1967-1998
NEWS 13	SEP 17	CAplus coverage extended to include traditional medicine patents
NEWS 14	SEP 24	EMBASE, EMBAL, and LEMBASE reloaded with enhancements
NEWS 15	OCT 02	CA/CAplus enhanced with pre-1907 records from Chemisches Zentralblatt
NEWS 16	OCT 19	BEILSTEIN updated with new compounds
NEWS 17	NOV 15	Derwent Indian patent publication number format enhanced
NEWS 18	NOV 19	WPIX enhanced with XML display format
NEWS 19	NOV 30	ICSD reloaded with enhancements
NEWS 20	DEC 04	LINPADOCDB now available on STN
NEWS 21	DEC 14	BEILSTEIN pricing structure to change
NEWS 22	DEC 17	USPATOLD added to additional database clusters
NEWS 23	DEC 17	IMSDRUGCONF removed from database clusters and STN
NEWS 24	DEC 17	DGENE now includes more than 10 million sequences
NEWS 25	DEC 17	TOXCENTER enhanced with 2008 MeSH vocabulary in MEDLINE segment
NEWS 26	DEC 17	MEDLINE and LMEDLINE updated with 2008 MeSH vocabulary
NEWS 27	DEC 17	CA/CAplus enhanced with new custom IPC display formats
NEWS 28	DEC 17	STN Viewer enhanced with full-text patent content from USPATOLD
NEWS 29	JAN 02	STN pricing information for 2008 now available
NEWS 30	JAN 16	CAS patent coverage enhanced to include exemplified prophetic substances
NEWS 31	JAN 28	USPATFULL, USPAT2, and USPATOLD enhanced with new custom IPC display formats
NEWS 32	JAN 28	MARPAT searching enhanced
NEWS 33	JAN 28	USGENE now provides USPTO sequence data within 3 days of publication
NEWS 34	JAN 28	TOXCENTER enhanced with reloaded MEDLINE segment

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 NEWS 35  JAN 28  MEDLINE and LMEDLINE reloaded with enhancements
 NEWS 36  FEB 08  STN Express, Version 8.3, now available


 NEWS EXPRESS FEBRUARY 08 CURRENT WINDOWS VERSION IS V8.3,
              AND CURRENT DISCOVER FILE IS DATED 24 JANUARY 2008

 NEWS HOURS    STN Operating Hours Plus Help Desk Availability
 NEWS LOGIN    Welcome Banner and News Items
 NEWS IPC8     For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that
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* * * * * * * * * * * * * * * STN  Columbus  * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 19:17:35 ON 19 FEB 2008

=> file reg
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                     0.21       0.21

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STRUCTURE FILE UPDATES:   18 FEB 2008  HIGHEST RN 1004360-55-7
DICTIONARY FILE UPDATES:  18 FEB 2008  HIGHEST RN 1004360-55-7

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 9, 2008.

  Please note that search-term pricing does apply when
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REGISTRY includes numerically searchable data for experimental and
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experimental property data in the original document.  For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Program Files\Stnexp\Queries\10518714b.str
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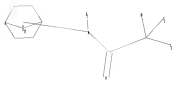


chain nodes :
11 12 13 14 17 18 20 21
ring nodes :
1 2 3 4 5 6 8
chain bonds :
11-12 11-14 12-13 12-17 17-18 17-20 17-21
ring bonds :
1-2 1-6 1-8 2-3 3-4 4-5 4-8 5-6
exact/norm bonds :
1-2 1-6 1-8 2-3 3-4 4-5 5-6 11-12 11-14 12-13 17-18 17-20 17-21
exact bonds :
4-8 12-17
isolated ring systems :
containing 1 : 17 :

G1:C,H

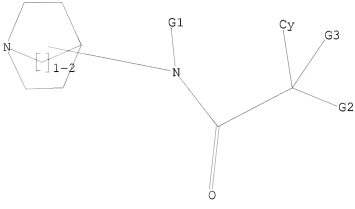
G2:C,H,OH

G3:C,Cy

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:Atom 11:CLASS 12:CLASS
13:CLASS 14:CLASS 16:CLASS 17:Atom 18:Atom 20:CLASS 21:CLASS

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR



G1 C,H

G2 C,H,OH

G3 C,Cy

Structure attributes must be viewed using STN Express query preparation.

=> s l1
SAMPLE SEARCH INITIATED 19:18:02 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 5748 TO ITERATE

34.8% PROCESSED 2000 ITERATIONS 1 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 110414 TO 119506
PROJECTED ANSWERS: 1 TO 158

L2 1 SEA SSS SAM L1

=> s l1 full
FULL SEARCH INITIATED 19:18:06 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 116546 TO ITERATE

100.0% PROCESSED 116546 ITERATIONS 88 ANSWERS
SEARCH TIME: 00.00.02

L3 88 SEA SSS FUL L1

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=> file caplus
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                   178.36     178.57

FILE 'CAPLUS' ENTERED AT 19:18:12 ON 19 FEB 2008
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FILE COVERS 1907 - 19 Feb 2008  VOL 148 ISS 8
FILE LAST UPDATED: 18 Feb 2008  (20080218/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:

http://www.cas.org/infopolicy.html

=> s l3 full
L4            9 L3

=> d ibib abs hitstr tot
```

L4 ANSWER 1 OF 9 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2005:528114 CAPLUS

DOCUMENT NUMBER: 143:259473

TITLE: A quantitative structure-activity relationship study on some Na+ and K+ channel blockers: Role of molecular connectivity index

AUTHOR(S): Gupta, S. P.; Paleti, Anitha; Mekapati, S. B.; Nagappa, A. N.; Kumaran, S.

CORPORATE SOURCE: Birla Institute of Technology and Science, Pilani, 333031, India

SOURCE: Letters in Drug Design & Discovery (2005), 2(4), 287-290
CODEN: LDDDAW; ISSN: 1570-1808

PUBLISHER: Bentham Science Publishers Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A quant. structure-activity relation (QSAR) study is made on a series of Na+ channel blockers (diphenylacetamide derivs.) and on a series of K+ channel blockers (blockers of cardiac delayed rectifier potassium current IKs) (benzodiazepine derivs.). In both the cases, the blocking activity is significantly correlated with Kier's first-order valence mol. connectivity index.

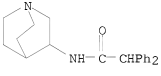
IT 739310-56-6

RL: PAC (Pharmacological activity); PRP (Properties); BIOL (Biological study)

(QSAR study on Na+ and K+ channel blockers: role of mol. connectivity index)

RN 739310-56-6 CAPLUS

CN Benzeneacetamide, N-1-azabicyclo[2.2.2]oct-3-yl-α-phenyl- (CA INDEX NAME)



REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 9 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2004:41467 CAPLUS
DOCUMENT NUMBER: 140:94180
TITLE: Preparation of new quinuclidine amide derivatives for therapeutic uses as antagonists of M3 muscarinic receptors
INVENTOR(S): Prat Quinones, Maria
PATENT ASSIGNEE(S): Almirall Prodesfarma S.A., Spain
SOURCE: PCT Int. Appl., 65 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004005285	A1	20040115	WO 2003-EP6708	20030625
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
ES 2204295	A1	20040416	ES 2002-1539	20020702
ES 2204295	B1	20050801		
CA 2492535	A1	20040115	CA 2003-2492535	20030625
AU 2003242757	A1	20040123	AU 2003-242757	20030625
EP 1519933	A1	20050406	EP 2003-762514	20030625
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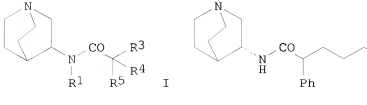
BR 2003012216	A	20050412	BR 2003-12216	20030625
CN 1678610	A	20051005	CN 2003-820648	20030625
JP 2005533826	T	20051110	JP 2004-518575	20030625
NZ 537341	A	20060428	NZ 2003-537341	20030625
RU 2314306	C2	20080110	RU 2005-102585	20030625
MX 2004PA12271	A	20050408	MX 2004-PA12271	20041207
ZA 2004010404	A	20050905	ZA 2004-10404	20041223
IN 2004DN04140	A	20061229	IN 2004-DN4140	20041227
NO 2005000164	A	20050404	NO 2005-164	20050112
US 2006167042	A1	20060727	US 2005-518714	20050801

PRIORITY APPLN. INFO.:			ES 2002-1539	A	20020702
			WO 2003-EP6708	W	20030625

OTHER SOURCE(S): MARPAT 140:94180
GI



AB N-quinuclidinyl amides, such as I [R1 = H, alkyl; R3 = furyl, thienyl, phenyl; R4 = alkyl, alkenyl, alkynyl, cycloalkyl, cycloalkylmethyl, Ph,

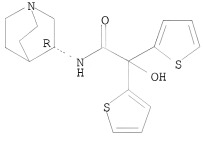
benzyl, phenethyl, furyl, thienyl; R5 = H, OH, Me, CH2OH], were prepared for use in therapy as antagonists of M3 muscarinic receptors. These amides are claimed for use in the treatment of respiratory, urol. or gastrointestinal pathol. conditions and diseases susceptible to amelioration by antagonism of M3 muscarinic receptors. Thus, amide II was prepared in 63.1% yield via an amidation reaction of (3R)-aminoquinuclidine with 2-phenylhexanoic acid in DMF and CHCl3. The prepared N-quinuclidinyl amides were assayed for human muscarinic receptor binding activity and for effect on bronchial response to i.v. acetylcholine challenge in guinea pigs. Tablet, liquid inhalant, powder inhalant, and inhalation aerosol pharmaceutical compns. of the amides were presented.

IT 644468-28-0P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of N-quinuclidinyl amides for use in pharmaceutical compns. as M3 muscarinic receptor antagonists)

RN 644468-28-0 CAPLUS

CN 2-Thiopheneacetamide, N-(3R)-1-azabicyclo[2.2.2]oct-3-yl-α-hydroxy-α-2-thienyl- (CA INDEX NAME)

Absolute stereochemistry.



IT 644468-21-3P 644468-24-6P 644468-26-8P
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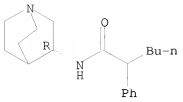
644469-07-8P 644469-08-9P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of N-quinuclidinyl amides for use in pharmaceutical compns. as M3 muscarinic receptor antagonists)

RN 644468-21-3 CAPLUS

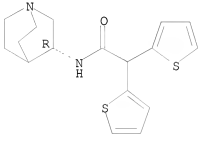
CN Benzeneacetamide, N-(3R)-1-azabicyclo[2.2.2]oct-3-yl-α-butyl- (CA INDEX NAME)

Absolute stereochemistry.



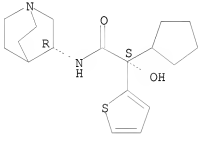
RN 644468-24-6 CAPLUS
CN 2-Thiopheneacetamide, N-(3R)-1-azabicyclo[2.2.2]oct-3-yl-α-2-thienyl-
(CA INDEX NAME)

Absolute stereochemistry.



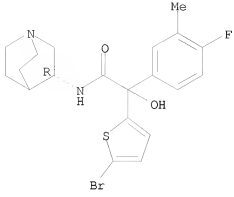
RN 644468-26-8 CAPLUS
CN 2-Thiopheneacetamide, N-(3R)-1-azabicyclo[2.2.2]oct-3-yl-α-
cyclopentyl-α-hydroxy-, (αS)- (CA INDEX NAME)

Absolute stereochemistry.



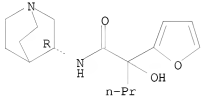
RN 644468-29-1 CAPLUS
CN 2-Thiopheneacetamide, N-(3R)-1-azabicyclo[2.2.2]oct-3-yl-5-bromo-α-
(4-fluoro-3-methylphenyl)-α-hydroxy- (CA INDEX NAME)

Absolute stereochemistry.



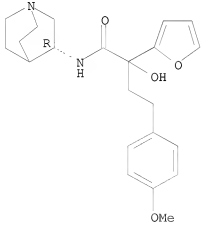
RN 644468-31-5 CAPLUS
CN 2-Furanacetamide, N-(3R)-1-azabicyclo[2.2.2]oct-3-yl-α-hydroxy-α-propyl- (CA INDEX NAME)

Absolute stereochemistry.



RN 644468-33-7 CAPLUS
CN 2-Furanacetamide, N-(3R)-1-azabicyclo[2.2.2]oct-3-yl-α-hydroxy-α-[2-(4-methoxyphenyl)ethyl]- (CA INDEX NAME)

Absolute stereochemistry.

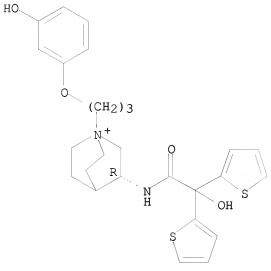


RN 644468-42-8 CAPLUS
CN 1-Azoniabicyclo[2.2.2]octane, 3-[(hydroxydi-2-thienylacetyl)amino]-1-[3-(3-hydroxyphenoxy)propyl]-, (3R)-, salt with trifluoroacetic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 644468-41-7
CMF C26 H31 N2 O4 S2

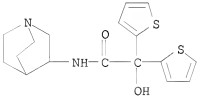
Absolute stereochemistry.



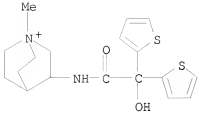
CM 2

CRN 14477-72-6
CMF C2 F3 O2

RN 644468-44-0 CAPLUS
CN 2-Thiopheneacetamide, N-1-azabicyclo[2.2.2]oct-3-yl-α-hydroxy-α-2-thienyl- (CA INDEX NAME)

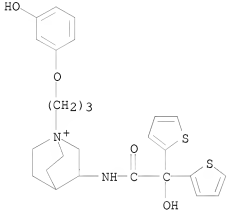


RN 644468-45-1 CAPLUS
CN 1-Azoniabicyclo[2.2.2]octane, 3-[(hydroxydi-2-thienylacetyl)amino]-1-methyl-, bromide (9CI) (CA INDEX NAME)



● Br^-

RN 644468-46-2 CAPLUS
CN 1-Azoniabicyclo[2.2.2]octane, 3-[(hydroxydi-2-thienylacetyl)amino]-1-[3-(3-hydroxyphenoxy)propyl]-, bromide (9CI) (CA INDEX NAME)



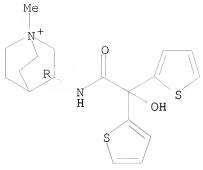
● Br^-

RN 644468-48-4 CAPLUS
CN 1-Azoniabicyclo[2.2.2]octane, 3-[(hydroxydi-2-thienylacetyl)amino]-1-methyl-, (3R)-, salt with trifluoroacetic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 644468-47-3
CMF C18 H23 N2 O2 S2

Absolute stereochemistry.



CM 2

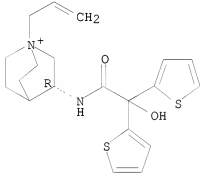
CRN 14477-72-6
CMF C2 F3 O2

RN 644468-50-8 CAPLUS
CN 1-Azoniabicyclo[2.2.2]octane, 3-[(hydroxydi-2-thienylacetyl)amino]-1-(2-propenyl)-, (3R)-, salt with trifluoroacetic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 644468-49-5
CMF C20 H25 N2 O2 S2

Absolute stereochemistry.



CM 2

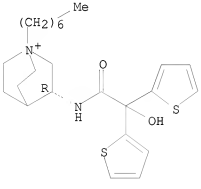
CRN 14477-72-6
CMF C2 F3 O2

RN 644468-52-0 CAPLUS
CN 1-Azoniabicyclo[2.2.2]octane, 1-heptyl-3-[(hydroxydi-2-thienylacetyl)amino]-, (3R)-, salt with trifluoroacetic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 644468-51-9
CMF C24 H35 N2 O2 S2

Absolute stereochemistry.

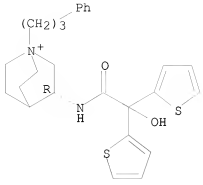


CM 2

CRN 14477-72-6
CMF C2 F3 O2

RN 644468-53-1 CAPLUS
CN 1-Azoniabicyclo[2.2.2]octane, 3-[(hydroxydi-2-thienylacetyl)amino]-1-(3-phenylpropyl)-, bromide, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



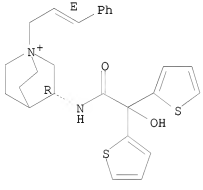
● Br^-

RN 644468-55-3 CAPLUS
CN 1-Azoniabicyclo[2.2.2]octane, 3-[(hydroxydi-2-thienylacetyl)amino]-1-[(2E)-3-phenyl-2-propenyl]-, (3R)-, salt with trifluoroacetic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 644468-54-2
CMF C26 H29 N2 O2 S2

Absolute stereochemistry.
Double bond geometry as shown.

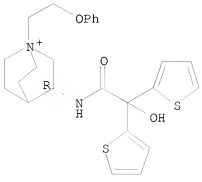


CM 2

CRN 14477-72-6
CMF C2 F3 O2

RN 644468-56-4 CAPLUS
CN 1-Azoniabicyclo[2.2.2]octane, 3-[(hydroxydi-2-thienylacetyl)amino]-1-(2-phenoxyethyl)-, bromide, (3R)- (9CI) (CA INDEX NAME)

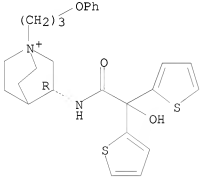
Absolute stereochemistry.



● Br⁻

RN 644468-57-5 CAPLUS
CN 1-Azoniabicyclo[2.2.2]octane, 3-[(hydroxydi-2-thienylacetyl)amino]-1-(3-phenoxypropyl)-, bromide, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



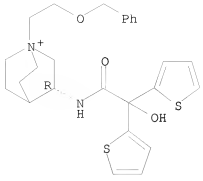
● Br⁻

RN 644468-59-7 CAPLUS
CN 1-Azoniabicyclo[2.2.2]octane, 3-[(hydroxydi-2-thienylacetyl)amino]-1-[2-(phenylmethoxy)ethyl]-, (3R)-, salt with trifluoroacetic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 644468-58-6
CMF C26 H31 N2 O3 S2

Absolute stereochemistry.

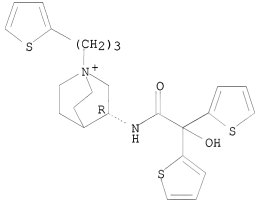


CM 2

CRN 14477-72-6
CMF C2 F3 O2

RN 644468-60-0 CAPLUS
CN 1-Azoniabicyclo[2.2.2]octane, 3-[(hydroxydi-2-thienylacetyl)amino]-1-[3-(2-thienyl)propyl]-, bromide, (3R)- (9CI) (CA INDEX NAME)

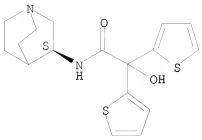
Absolute stereochemistry.



● Br⁻

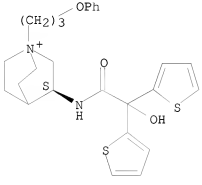
RN 644468-61-1 CAPLUS
CN 2-Thiopheneacetamide, N-(3S)-1-azabicyclo[2.2.2]oct-3-yl-α-hydroxy-α-2-thienyl- (CA INDEX NAME)

Absolute stereochemistry.



RN 644468-62-2 CAPLUS
CN 1-Azoniabicyclo[2.2.2]octane, 3-[(hydroxydi-2-thienylacetyl)amino]-1-(3-phenoxypropyl)-, bromide, (3S)- (9CI) (CA INDEX NAME)

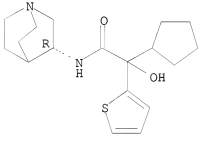
Absolute stereochemistry.



● Br⁻

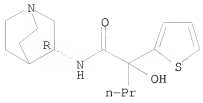
RN 644468-63-3 CAPLUS
CN 2-Thiopheneacetamide, N-(3R)-1-azabicyclo[2.2.2]oct-3-yl-α-cyclopentyl-α-hydroxy- (CA INDEX NAME)

Absolute stereochemistry.



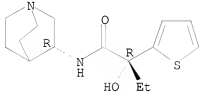
RN 644468-64-4 CAPLUS
CN 2-Thiopheneacetamide, N-(3R)-1-azabicyclo[2.2.2]oct-3-yl-α-hydroxy-α-propyl- (CA INDEX NAME)

Absolute stereochemistry.



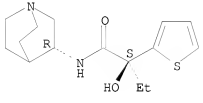
RN 644468-65-5 CAPLUS
CN 2-Thiopheneacetamide, N-(3R)-1-azabicyclo[2.2.2]oct-3-yl-α-ethyl-α-hydroxy-, (αR)- (CA INDEX NAME)

Absolute stereochemistry.



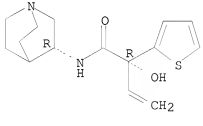
RN 644468-66-6 CAPLUS
CN 2-Thiopheneacetamide, N-(3R)-1-azabicyclo[2.2.2]oct-3-yl-α-ethyl-α-hydroxy-, (αS)- (CA INDEX NAME)

Absolute stereochemistry.



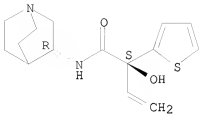
RN 644468-67-7 CAPLUS
CN 2-Thiopheneacetamide, N-(3R)-1-azabicyclo[2.2.2]oct-3-yl-α-ethenyl-α-hydroxy-, (αR)- (CA INDEX NAME)

Absolute stereochemistry.



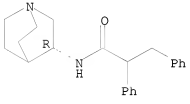
RN 644468-68-8 CAPLUS
CN 2-Thiopheneacetamide, N-(3R)-1-azabicyclo[2.2.2]oct-3-yl-α-ethenyl-α-hydroxy-, (αS)- (CA INDEX NAME)

Absolute stereochemistry.



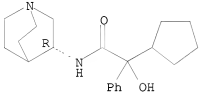
RN 644468-69-9 CAPLUS
CN Benzenepropanamide, N-(3R)-1-azabicyclo[2.2.2]oct-3-yl-α-phenyl-
(CA INDEX NAME)

Absolute stereochemistry.



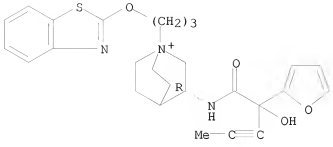
RN 644468-70-2 CAPLUS
CN Benzeneacetamide, N-(3R)-1-azabicyclo[2.2.2]oct-3-yl-α-cyclopentyl-
α-hydroxy- (CA INDEX NAME)

Absolute stereochemistry.



RN 644468-86-0 CAPLUS
CN 1-Azoniabicyclo[2.2.2]octane, 1-[3-(2-benzothiazolyloxy)propyl]-3-[[2-(2-
furanyl)-2-hydroxy-1-oxo-3-pentynyl]amino]-, chloride, (3R)- (9CI) (CA
INDEX NAME)

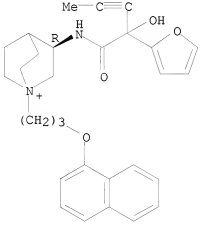
Absolute stereochemistry.



● Cl⁻

RN 644468-87-1 CAPLUS
CN 1-Azoniabicyclo[2.2.2]octane, 3-[[2-(2-furanyl)-2-hydroxy-1-oxo-3-pentynyl]amino]-1-[3-(1-naphthalenyloxy)propyl]-, chloride, (3R)- (9CI) (CA INDEX NAME)

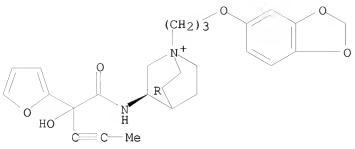
Absolute stereochemistry.



● Cl⁻

RN 644468-88-2 CAPLUS
CN 1-Azoniabicyclo[2.2.2]octane, 1-[3-(1,3-benzodioxol-5-yloxy)propyl]-3-[[2-(2-furanyl)-2-hydroxy-1-oxo-3-pentynyl]amino]-, bromide, (3R)- (9CI) (CA INDEX NAME)

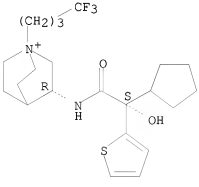
Absolute stereochemistry.



● Br^-

RN 644468-89-3 CAPLUS
CN 1-Azoniabicyclo[2.2.2]octane, 3-[[(2S)-cyclopentylhydroxy-2-thienylacetyl]amino]-1-(4,4,4-trifluorobutyl)-, bromide, (3R)- (9CI) (CA INDEX NAME)

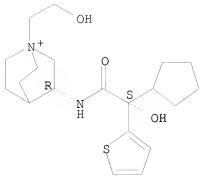
Absolute stereochemistry.



● Br^-

RN 644468-90-6 CAPLUS
CN 1-Azoniabicyclo[2.2.2]octane, 3-[[(2S)-cyclopentylhydroxy-2-thienylacetyl]amino]-1-(2-hydroxyethyl)-, bromide, (3R)- (9CI) (CA INDEX NAME)

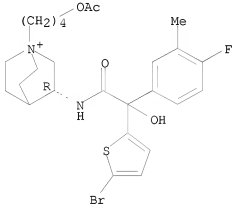
Absolute stereochemistry.



● Br⁻

RN 644468-91-7 CAPLUS
CN 1-Azoniabicyclo[2.2.2]octane, 1-[4-(acetyloxy)butyl]-3-[[(5-bromo-2-thienyl)(4-fluoro-3-methylphenyl)hydroxyacetyl]amino]-, bromide, (3R)-(9CI) (CA INDEX NAME)

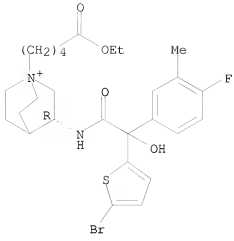
Absolute stereochemistry.



● Br⁻

RN 644468-92-8 CAPLUS
CN 1-Azoniabicyclo[2.2.2]octane, 3-[[(5-bromo-2-thienyl)(4-fluoro-3-methylphenyl)hydroxyacetyl]amino]-1-(5-ethoxy-5-oxopentyl)-, bromide, (3R)- (9CI) (CA INDEX NAME)

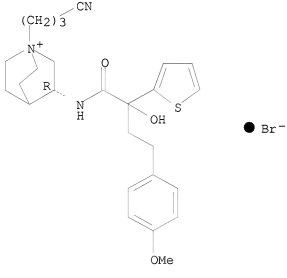
Absolute stereochemistry.



● Br^-

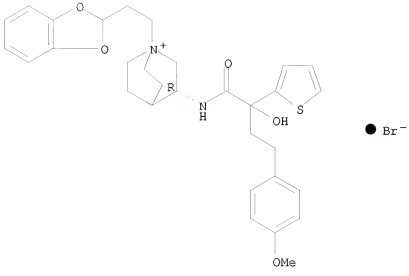
RN 644468-93-9 CAPLUS
CN 1-Azoniabicyclo[2.2.2]octane, 1-(3-cyanopropyl)-3-[[2-hydroxy-4-(4-methoxyphenyl)-1-oxo-2-(2-thienyl)butyl]amino]-, bromide, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 644468-94-0 CAPLUS
CN 1-Azoniabicyclo[2.2.2]octane, 1-[2-(1,3-benzodioxol-2-yl)ethyl]-3-[[2-hydroxy-4-(4-methoxyphenyl)-1-oxo-2-(2-thienyl)butyl]amino]-, bromide, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

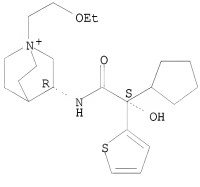


RN 644469-05-6 CAPLUS
CN 1-Azoniabicyclo[2.2.2]octane, 3-[[(2S)-cyclopentylhydroxy-2-thienylacetyl]amino]-1-(2-ethoxyethyl)-, (3R)-, formate (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 644469-04-5
CMF C22 H35 N2 O3 S

Absolute stereochemistry.



CM 2

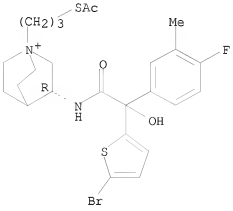
CRN 71-47-6
CMF C H O2

RN 644469-07-8 CAPLUS
CN 1-Azoniabicyclo[2.2.2]octane, 1-[3-(acetylthio)propyl]-3-[[(5-bromo-2-thienyl)(4-fluoro-3-methylphenyl)hydroxyacetyl]amino]-, (3R)-, formate (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 644469-06-7
CMF C25 H31 Br F N2 O3 S2

Absolute stereochemistry.

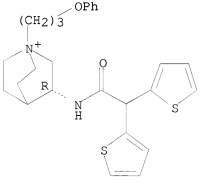


CM 2

CRN 71-47-6
CMF C H O2

RN 644469-08-9 CAPLUS
CN 1-Azoniabicyclo[2.2.2]octane, 3-[(di-2-thienylacetyl)amino]-1-(3-phenoxypropyl)-, bromide, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● Br−

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1998:8644 CAPLUS
DOCUMENT NUMBER: 128:102011
TITLE: Preparation of pyridylacetamides as anticholinergics for treatment of pollakiuria and urinary incontinence
INVENTOR(S): Taniguchi, Kiyoshi; Tsubaki, Kazunori
PATENT ASSIGNEE(S): Fujisawa Pharmaceutical Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 13 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 09328469	A	19971222	JP 1997-55064	19970310
PRIORITY APPLN. INFO.:			AU 1996-8629 A	19960313
OTHER SOURCE(S):		MARPAT 128:102011		

GI

II

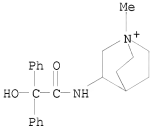
III

IV

AB R2CR1R3CONR10(A)nR4 (I; R1, R2 = aryl; R3 = OH, halo; R4 = II, III, IV; B = N, NR5+X-; C = NR6, NR7R8+Y-; R5 = lower alkyl, imino-protecting group; X-, Y-, Z- = anion; R6 = H, lower alkyl, imino-protecting group; doted line = optional single bond; R7, R8, R9 = lower alkyl; R10 = H, lower alkyl, A = lower alkylene; n = 0, 1; if R10 = H, then II (B = N or NR5+X-) or III (C = NR6) is bonded at 3-position) and their pharmaceutically acceptable salts are prepared 2-Hydroxy-N-methyl-2,2-diphenyl-N-[[1,2,3,6-tetrahydro-1-(4-methoxybenzyl)-4-pyridyl]methyl]acetamide (1.60 g) was deprotected using ClCO2CHClMe in ClCH2CH2Cl-MeOH under reflux for 50 min and reacted with HCl in AcOEt to give 695 mg I (R1 = R2 = Ph, R3 = OH, R10 = Me, R4 = 1,2,3,6-tetrahydro-4-pyridyl, A = CH2, n = 1) (V). V showed ED30 of 0.0056 mg/kg in inhibition of urinary bladder contractions in rats.

IT 201340-53-6P 201340-54-7P 201340-55-8P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyridylacetamides as anticholinergics for treatment of pollakiuria and urinary incontinence)

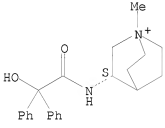
RN 201340-53-6 CAPLUS
CN 1-Azoniabicyclo[2.2.2]octane, 3-[(hydroxydiphenylacetyl)amino]-1-methyl-, iodide (9CI) (CA INDEX NAME)



● I⁻

RN 201340-54-7 CAPLUS
CN 1-Azoniabicyclo[2.2.2]octane, 3-[(hydroxydiphenylacetyl)amino]-1-methyl-, bromide, (S)- (9CI) (CA INDEX NAME)

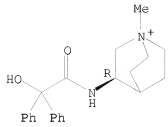
Absolute stereochemistry.



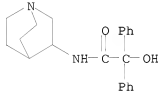
● Br⁻

RN 201340-55-8 CAPLUS
CN 1-Azoniabicyclo[2.2.2]octane, 3-[(hydroxydiphenylacetyl)amino]-1-methyl-, bromide, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

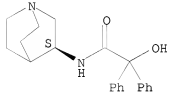


IT 201340-52-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of pyridylacetamides as anticholinergics for treatment of pollakiuria and urinary incontinence)
RN 201340-52-5 CAPLUS
CN Benzeneacetamide, N-1-azabicyclo[2.2.2]oct-3-yl-α-hydroxy-α-phenyl- (CA INDEX NAME)



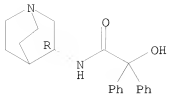
IT 201340-42-3P 201340-43-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of pyridylacetamides as anticholinergics for treatment of pollakiuria and urinary incontinence)
RN 201340-42-3 CAPLUS
CN Benzeneacetamide, N-1-azabicyclo[2.2.2]oct-3-yl-α-hydroxy-α-phenyl-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 201340-43-4 CAPLUS
CN Benzeneacetamide, N-1-azabicyclo[2.2.2]oct-3-yl-α-hydroxy-α-phenyl-, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

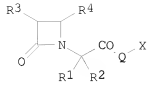

N
R
O
OH
N
H
Ph
Ph

L4 ANSWER 4 OF 9 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1997:576686 CAPLUS
DOCUMENT NUMBER: 127:234215
TITLE: Preparation of non-peptidyl vasopressin V1a receptor antagonists
INVENTOR(S): Bruns, Robert F., Jr.; Cooper, Robin D. G.; Dressman, Bruce A.; Hunden, David C.; Kaldor, Stephen W.; Koppel, Gary A.; Rizzo, John R.; Skelton, Jeffrey James; et al.
PATENT ASSIGNEE(S): Eli Lilly and Co., USA; Bruns, Robert F., Jr.; Cooper, Robin D. G.; Dressman, Bruce A.; Hunden, David C.; Kaldor, Stephen W.; Koppel, Gary A.
SOURCE: PCT Int. Appl., 158 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

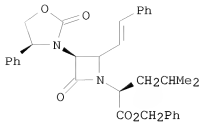
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9730707	A1	19970828	WO 1997-US3039	19970220
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
CA 2246753	A1	19970828	CA 1997-2246753	19970220
CA 2246753	C	20050510		
AU 9719779	A	19970910	AU 1997-19779	19970220
EP 939632	A1	19990908	EP 1997-907895	19970220
EP 939632	B1	20051005		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, NL, SE, PT, IE, FI				
JP 2000504731	T	20000418	JP 1997-529647	19970220
AT 305781	T	20051015	AT 1997-907895	19970220
ES 2248840	T3	20060316	ES 1997-907895	19970220
US 6204260	B1	20010320	US 1999-125737	19990819
US 2002049187	A1	20020425	US 2000-733430	20001208
US 6521611	B2	20030218		
US 6610680	B1	20030826	US 2002-327240	20021220

PRIORITY APPLN. INFO.:	US 1996-12149P	P	19960223
	US 1996-12188P	P	19960223
	US 1996-12215P	P	19960223
	GB 1996-5044	A	19960309
	GB 1996-5045	A	19960309
	GB 1996-5046	A	19960309
	WO 1997-US3039	W	19970220
	US 1999-125737	A3	19990819
	US 2000-733430	A3	20001208

OTHER SOURCE(S): MARPAT 127:234215
GI



I



II

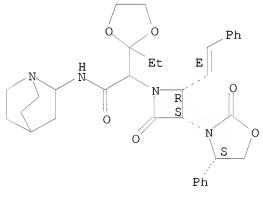
AB Azetidinones I [R1 = H, alkyl, carbamoyl, alkoxy, acyl, benzoyl, phenyl; R2 = H, OH, alkyl; R3 = phthalimido, azido, phenoxyacetamido, oxazolinyl, imidazolinyl, pyrrolidinyl, ureido; Q = O, S, NR5; X = H, alkyl; R5 = H, alkyl, OH, alkoxycarbonyl, benzyl] were prepared for use as vasopressin V1a receptor antagonists. Thus, azetidinone II was prepared starting from L-leucine benzyl ester, cinnamaldehyde, and 2-[4(S)-phenyloxazolidin-2-on-3-yl]acetyl chloride. II gave an IC50 value of 39 nM when tested for vasopressin V1a receptor binding affinity.

IT 195309-73-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of non-peptidyl vasopressin V1a receptor antagonists)

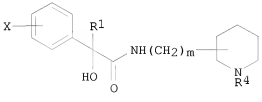
RN 195309-73-0 CAPLUS

CN 1-Azetidineacetamide, N-1-azabicyclo[2.2.2]oct-2-yl-α-(2-ethyl-1,3-dioxolan-2-yl)-2-oxo-3-(2-oxo-4-phenyl-3-oxazolidinyl)-4-(2-phenylethenyl)-, [3S-[3α(R*),4α(E)]]-[partial]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



L4 ANSWER 5 OF 9 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1995:6185 CAPLUS
DOCUMENT NUMBER: 122:81073
TITLE: Agents for the treatment of overactive detrusor. VI. Synthesis and pharmacological properties of acetamide derivatives bearing cyclic amines in N-substituents
AUTHOR(S): Taniguchi, Kiyoshi; Tsubaki, Kazunori; Mizuno, Hiroaki; Take, Kazuhiko; Okumura, Kazuo; Terai, Takao; Shiokawa, Youichi
CORPORATE SOURCE: New Drug. Res. Lab., Fujisawa Pharm. Co., Ltd., Osaka, 532, Japan
SOURCE: Chemical & Pharmaceutical Bulletin (1994), 42(1), 74-84
CODEN: CPBTAL; ISSN: 0009-2363
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



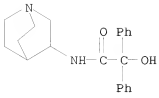
I

AB With the aim of improving the efficacy and decreasing the efficacy and decreasing the side effects of oxybutynin, N-[(tetrahydro-3-pyridyl)methyl]- or N-[(tetrahydro-4-pyridyl)methyl]-, N-(4-piperidyl)-, and N-(3-piperidylalkyl)- or N-(4-piperidylalkyl)-2-hydroxyacetamides (such as) I (X = H, halo, etc.; R1 = cyclohexyl, Ph, etc.; R4 = H, alkyl, etc.) and related carboxamides were prepared and evaluated for inhibitory activity against urinary bladder rhythmic contraction in rats and for mydriatic activity in rats. Some of these compds. were superior to oxybutynin in both inhibitory activity against bladder contraction and selectivity between inhibitory activity against bladder contraction and mydriatic activity. Judging from the effect of I (X = H, R1 = Ph, R4 = H) on detrusor contraction in vivo in guinea-pigs, it appeared that the inhibitory activity of I against bladder contraction in vivo was related mainly to its inhibitory activity against detrusor contraction in vitro induced with carbacol (antimuscarine-like activity). The selectivity (20-fold) of I between inhibitory activity against bladder contraction and mydriatic activity was greatly superior to that (0.48-fold) of oxybutynin. Compound I was prepared by debenzylation of the corresponding N-[[1-(4-methoxybenzyl)-tetrahydro-4-pyridyl]methyl] derivative

IT 153196-23-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, for treatment of urinary frequency or incontinence)

RN 153196-23-7 CAPLUS

CN Benzeneacetamide, N-1-azabicyclo[2.2.2]oct-3-yl-α-hydroxy-α-phenyl-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

L4 ANSWER 6 OF 9 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1994:163981 CAPLUS
DOCUMENT NUMBER: 120:163981
TITLE: Preparation of substituted acetamides for treatment of bladder disorders
INVENTOR(S): Shiokawa, Youichi; Taniguchi, Kiyoshi; Take, Kazuhiko; Tsubaki, Kazunori; Mizuno, Hiroaki
PATENT ASSIGNEE(S): Fujisawa Pharmaceutical Co., Ltd., Japan
SOURCE: PCT Int. Appl.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9316048	A1	19930819	WO 1993-JP142	19930204

W: CA, JP, KR, US
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE

PRIORITY APPLN. INFO.: GB 1992-2443 A 19920205
OTHER SOURCE(S): MARPAT 120:163981
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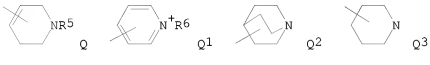

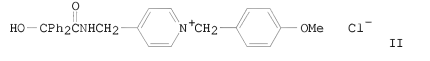

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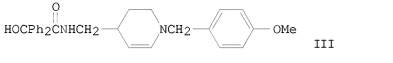


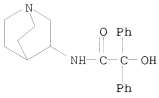
III

AB Title compds. R1R2R3C(A1)mCONH(A2)nR4 [I; R1, R2 = (un)substituted aryl; R3 = H, OH, alkyl; R4 = Q, Q1, Q2, Q3; R5 = Me, Et, Pr, iso-Pr, protecting group; R6 = alkyl; R7 = alkyl, protecting group; A1, A2 = alkylene; m, n = 0, 1; with provisos] are prepared HOCPh2CONHCH2Q4 [Q4 = 4-pyridyl] (preparation given) was treated with p-MeOC6H4CH2Cl to give the quaternary ammonium compound II, which was reduced with NaBH4 in MeOH and the resulting tetrahydropyrinde derivative III was refluxed with ClCO2CHClMe in CH2Cl2 to give, after treatment with 4N HCl, the title compound I.HCl [R1 = R2 = Ph, R3 = OH, A1 = bond, A2 = CH2, R4 = 1,2,3,4-tetrahydro-4-pyridyl]. The tested I had an IC30 of 0.005 mg/Kg s.c. in controlling bladder contraction in rats.

IT 153196-23-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, for treatment of bladder disorders)

RN 153196-23-7 CAPLUS

CN Benzeneacetamide, N-1-azabicyclo[2.2.2]oct-3-yl-α-hydroxy-α-phenyl-, monohydrochloride (9CI) (CA INDEX NAME)

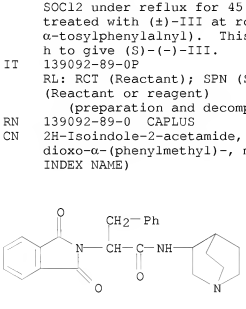


● HCl

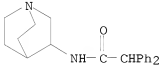
L4 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1992:106123 CAPLUS
DOCUMENT NUMBER: 116:106123
TITLE: 3-(N-substituted-amino)quinuclidines and preparation of optically active 3-aminoquinuclidine therefrom
INVENTOR(S): Kawakita, Takeshi; Sano, Mitsuharu; Kuroita, Takanobu; Ikezawa, Ryuhei
PATENT ASSIGNEE(S): Yoshitomi Pharmaceutical Industries, Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 6 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 03218376	A	19910925	JP 1990-307953	19901113
PRIORITY APPLN. INFO.:			JP 1989-296938	A1 19891114

OTHER SOURCE(S): MARPAT 116:106123
GI For diagram(s), see printed CA Issue.
AB 3-Aminoquinuclidines I (R = N-protected amino acid residue) (II) and optically active II and a process for the preparation of optically active I (R = H) (III) by treatment of optically active N-protected amino acids with racemic III, followed by separation of the resultant diastereomeric II and hydrolysis. (S)-α-Tosylphenylalanine in CHCl3 was treated with SOCl2 under reflux for 45 min and the resultant acid chloride in CHCl3 was treated with (±)-III at room temperature for 30 min to give (S,S)-II.HCl (R = α-tosylphenylalnyl). This was treated with H2SO4 under reflux for 4 h to give (S)-(-)-III.
IT 139092-89-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and decomposition of)
RN 139092-89-0 CAPLUS
CN 2H-Isoindole-2-acetamide, N-1-azabicyclo[2.2.2]oct-3-yl-1,3-dihydro-1,3-dioxo-α-(phenylmethyl)-, monohydrochloride, [S-(R*,S*)]- (9CI) (CA INDEX NAME)



L4 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1973:546358 CAPLUS
DOCUMENT NUMBER: 79:146358
ORIGINAL REFERENCE NO.: 79:23717a,23720a
TITLE: Synthesis and pharmacological study of 3-hydroxy- and 3-aminoquinuclidine derivatives
AUTHOR(S): Mikhlina, E. E.; Zaitseva, K. A.; Vorob'eva, V. Ya.; Mashkovskii, M. D.; Yakhontov, L. N.
CORPORATE SOURCE: Vses. Nauchno-Issled. Khim.-Farm. Inst. im. Ordzhonikidze, Moscow, USSR
SOURCE: Khimiko-Farmatsevticheskii Zhurnal (1973), 7(8), 20-4
CODEN: KHFZAN; ISSN: 0023-1134
DOCUMENT TYPE: Journal
LANGUAGE: Russian
GI For diagram(s), see printed CA Issue.
AB 3-Hydroxyquinuclidine reacted with 2,3,4-RR1R2C6H2COCl (R = HO, NO2, Me, Cl, Br, H; R1 = H, Me; R2 = H, Cl, Me) (8 compds.) to give the corresponding (benzoyloxy)quinuclidines I. N-Quinuclidinyl amides II (R3 = 4-O2NC6H4, PhCH2, PhCH2CH2, Ph2CH, 4-ClC6H4OCH2, 2,4-Cl2C6H3) were prepared by condensation of 3-aminoquinuclidine with R3COCl. 3-Oxoquinoline reacted with HOCH2CH2NH2 and was then hydrogenated to give (ethylamino)quinuclidine III (R = H; R1 = HO), which underwent methylation and then chlorination to give III (R = Me; R1 = Cl). The latter reacted with morpholine and 1-methylpiperazine to give III (R = Me; R1 = morpholino, 4-methyl-1-piperazinyl). Cyanoethylation of 3-(methylamino)quinuclidine yielded III (R = Me, R1 = CN). Amides II possessed narcotic, nerve center blocking, and hypotensive activity.
IT 50684-14-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation, nerve center blocking and hypotensive activity of)
RN 50684-14-5 CAPLUS
CN Benzeneacetamide, N-1-azabicyclo[2.2.2]oct-3-yl-α-phenyl-, monohydrochloride (9CI) (CA INDEX NAME)

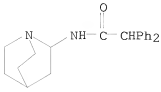


● HCl

L4 ANSWER 9 OF 9 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1954:35976 CAPLUS
DOCUMENT NUMBER: 48:35976
ORIGINAL REFERENCE NO.: 48:6438f-i,6439a-d
TITLE: Antispasmodics. II. Esters of basic bicyclic alcohols
AUTHOR(S): Sternbach, L. H.; Kaiser, S.
CORPORATE SOURCE: Hoffmann-La Roche, Nutley, NJ
SOURCE: Journal of the American Chemical Society (1952), 74, 2219-21
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.
AB The 7 basic alcs., 3-quinuclidinol (I), 2-benzyl-3-quinuclidinol (II), 1-azabil cyclo[3.2.1]-6-octanol (III), 1-azabicyclo[3.3.1]-4-nonano-(IV), 1-azabicyclo[3.3.1]-2-methyl-4-nonanol (V), and octahydro-1-pyrrocolinol (VI), were esterified with Ph2CHCO2H (VII), and I and III with other related acids. Of the 17 compds. prepared (see below), 5 showed an antiacetylcholine activity equaling or surpassing that of atropine. Of the 2 enantiomorphic 3-diphenylacetyl quinuclidines derived from the optical antipodes of I, the l-isomer has the most antiacetylcholine activity, while the d-isomer shows very low potency; the toxicities of both isomers are equal. Other relationships between structure and activity are discussed. Preparation of esters. Procedure A: The acid chloride and alc. (0.05 mole each) in 300 cc. C6H6 refluxed 15 hrs., and the product held 24 hrs. at 5°, then filtered yielded the ester. Procedure B: The acid chloride and alc. (or diamine) in 300 cc. C6H6 were refluxed 15 hrs., the product was cooled, acidified with ice-cold HCl, the aqueous solution washed with C6H6 or Et2O, the base liberated with ice-cold alkali, and extracted with Et2O. Procedure C: The basic alc. was refluxed with Na in 50 cc. PhMe 2-4 hrs., the alcoholate cooled with ice, treated with Ph2CClCOCl in 20-40 cc. PhMe, the mixture stirred 1 hr. at room temperature, treated with iso-PrOH, 120 cc. N HCl added, the mixture refluxed 10 min., the aqueous phase made alkaline and extracted with Et2O or CH3Cl. Procedure D: Preparation of salts of the basic esters. A cold alc. solution of the ester was neutralized with the dilute acid. Procedure E: Mixture of tropic and atropic esters of I. Acetyltropyl chloride (from 3.32 g. of tropic acid) in 10 cc. C6H6 added to 2.6 g. I in 100 cc. C6H6, the mixture let stand 14 hrs. at room temperature, heated 2 hrs. at 50°, cooled, extracted with ice-cold dilute HCl, the aqueous solution made alkaline, the ester extracted with Et2O, the Et2O solution concentrated in vacuo, the residue in N alc. titrated with N NaOH (phenolphthalein) at 30-45°, the mixture diluted with water, extracted with Et2O, and the extract concentrated in vacuo to yield 2 g. of oil. Procedure F: Equivalent amts. of Ph2C(CH2CH:CH2)COCl (VIII) and Et2NCH2CH2Cl were refluxed 20 hrs. and the product isolated by procedures B and D. Procedure G: The mixture of esters from d- and dl-I with VII was resolved by fractional crystallization from petr. ether to give the d-ester, [α]25D 10.5° (c 3.3, 0.5N HCl); m.p. not depressed by mixture with the racemate. Procedure H: Free VI (from the picrate, cf. part I) was esterified by procedure B.

Base, Acid, Procedure, % Yield, M.p. °C., Activity(atropine = 1); I, VII, B, 86, 95-6, ; I, VII-sulfate, D, , 95-103, 1; l-I, VII, B, 80, 89-90, 2; d-I, VII, G + B, , 89-90, 1/12; I, Benzilic, C, 40-60, 164-5, ; I, Benzilic-HCl, D, , 239-41, 2; I, 9-Fluorenecarboxylic-HCl (IX), A, 90, 201-5, 2; I, Tropic + atropic, E, 40, Oil, 1/2; I, VIII, C + D, 50, 185-91, 1/25-1/50; (a), VIII, F, 50, 108-10, 1/500; II, VII, A, 50, 250-2, 1/40-1/25; III, VII, A, 80, 191-2, 1/2; III, IX, A, 84, 212-20, 1; IV, VII, A, 88, 214-16, 1/10; V, VII, A, 92, 188-90, 1/5-1/10; VI, VII, H, , 64-6, 1/100; (b), VII, B, , 177-9, <1/100; (a) Et2NCH2CH2OH. (b) 3-Aminoquinuclidine.

IT 860503-38-4P, Quinuclidine, 3-(2,2-diphenylacetamido)-
RL: PREP (Preparation)
(preparation of)
RN 860503-38-4 CAPLUS
CN Quinuclidine, 3-(2,2-diphenylacetamido)- (5CI) (CA INDEX NAME)



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L2               1 S L1
L3              88 S L1 FULL

     FILE 'CAPLUS' ENTERED AT 19:18:12 ON 19 FEB 2008
L4               9 S L3 FULL

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COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                    51.93     230.50

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                       ENTRY    SESSION
CA SUBSCRIBER PRICE                                    -7.20      -7.20

STN INTERNATIONAL LOGOFF AT 19:21:53 ON 19 FEB 2008
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